

Second-order dynamic transition in a $p = 2$ spin-glass model

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We consider the dynamics of a disordered p -spin model with $p = 2$, analyzing the dynamics within Ruelle’s thermodynamic formalism. We use an indicator of the dynamical activity to construct the relevant dynamical Gibbs ensemble. We prove that the dynamics in the low-temperature (spin glass) phase of the model take place at a second-order phase transition between dynamically active and inactive trajectories. We also show that the same behaviour is found in a related model of a three-dimensional ferromagnet.

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I. INTRODUCTION

Glassy systems are characterised by their dynamical properties: at their glass transitions, they fall out of equilibrium on experimental time-scales, and exhibit aging phenomena. As the glass transition is approached, their relaxation times increase in a super-Arrhenius fashion and the decay of their equilibrium dynamical correlation functions is slower than exponential [1]. In the last fifteen years, several approaches have been developed to recover theoretically the experimental, out-of-equilibrium results (see, for example, [2]).

One of the most striking experimental features of a glass-forming liquid is that the increase in relaxation time near the glass transition does not seem to be accompanied by any significant changes in the liquid structure. However, experiments and computer simulations [3, 4, 5, 6] both indicate that a *dynamical* length scale is growing as the glass transition is approached. That is, glassy materials are made up of active and inactive regions of space-time, namely *dynamical heterogeneities*. Based upon these results, the idea that the glassy properties of a system arise directly from their dynamical heterogeneity was developed in [7, 8], stimulating further theoretical understandings of glassy dynamics.

Spin glasses are magnetic spin systems which exhibit several features in common with glass-forming liquids. They are modelled by spins with quenched random interactions between them, and have been extensively investigated both experimentally and theoretically (see [9] for a review). The purpose of this paper is to show that the glassy dynamics of a particular spin glass model can be understood in terms of the histories it follows in configuration space. To this end, we employ the thermodynamic formalism of histories, developed by Ruelle and coworkers [10] within the framework of dynamical systems theory, and summarized in [11] in the context of Markov dynamics. While equilibrium statistical mechanics is concerned with fluctuations in the configuration space of the system, Ruelle’s formalism focuses on the trajectories (histories) by which the system evolves through configuration space. The method has been applied recently to kinet-

ically constrained models of glass-formers [12] and to a Lennard Jones binary mixture [13]. Both these studies distinguish *active* and *inactive* histories of the systems, according to the range of configuration space visited during the history. In the kinetically constrained models, it was proven that the active and inactive histories form distinct populations. In the language of the thermodynamic formalism, they are separated by a first-order phase transition in trajectory space. In Refs. [12, 13], it was argued that the heterogeneous dynamics of those models is intrinsically linked to this transition.

In this article, we focus on a soft p -spin model with $p = 2$, whose static and dynamic properties can be studied analytically. The $p \rightarrow \infty$ limit of the p -spin model, namely the disordered Random Energy Model, was recently shown to possess a connection between the activity of the histories it follows and the dynamical heterogeneities in its glassy phase [14]. (Of course, in p -spin models with infinite-ranged interactions, the dynamical correlation lengths associated with dynamical heterogeneity are ill-defined. However, the presence of large dynamical fluctuations in these mean-field models is naturally linked to dynamical heterogeneity in their finite-dimensional counterparts. We show that the $p = 2$ spin-glass model is closely related to a three-dimensional ferromagnet in which such length scales can be calculated.) In both the spin glass and ferromagnetic models, we demonstrate the existence of a phase transition in trajectory space, offering further evidence that these phase transitions are very generally associated with glassy systems.

The outline of the paper is as follows: in Section II we describe the models we will consider and the methods that we will use. In section III we construct a ‘dynamic phase diagram’ that describes the behaviour of the system in trajectory space. We interpret our results in Sec. IV, discussing the links between the large deviations that we have derived and the more familiar features of the soft spin models, and identifying directions for further study.

II. MODEL AND FORMALISM

A. Spin glass model

We consider a system of N continuous spins σ_i whose Hamiltonian \mathcal{H} is given by:

$$\beta\mathcal{H} = -\frac{\beta}{2N} \sum_{i,j} J_{ij} \sigma_i \sigma_j + \frac{u}{N} \sum_{i,j} \sigma_i^2 \sigma_j^2. \quad (1)$$

Here, $\beta = 1/T$ as usual, where T is the temperature and we have set Boltzmann's constant to unity, we take $u > 0$, and the random couplings are Gaussian distributed

$$p(J_{ij}) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{J_{ij}^2}{2}\right). \quad (2)$$

The role of the term proportional to $u > 0$ is to suppress configurations with extreme values of the spins. The model is similar to the p -spin models discussed in [15, 16]. Like the spherical p -spin model of [15] and in contrast to that of [16], the model under consideration here can be solved exactly. However, we use the u -term instead of a spherical constraint since it facilitates studies of large-deviations of the activity. (In particular, we note that fluctuations of extensive quantities require careful treatment in spherical models [17], in which fluctuations of the Lagrange multiplier for the constraint must be considered.) In any case, all of these soft p -spin models exhibit finite-temperature 'glass transitions' at which ergodicity is broken [16, 18, 19, 20]. Connections with the structural glass problem have been discussed in [16, 21, 22]. The case of $p = 2$ differs from that of $p \geq 3$ in that correlation functions can be obtained exactly from the properties of large random matrices [18].

In this article, we will employ the functional-integral formalism of [23]. To this end, we endow the spin system with a relaxational dynamics,

$$\partial_t \sigma_i = -\frac{\delta \beta \mathcal{H}}{\delta \sigma_i(t)} + \eta_i(t) \quad (3)$$

where the η_i 's are independent white Gaussian noises with variance 2. Following [18, 20], it will prove useful to resort to the basis which diagonalizes the matrix of exchange couplings. The eigenvalues $\{J_\mu\}_{\mu=1,\dots,N}$ of the $N \times N$ matrix $(J_{ij})_{i,j=1,\dots,N}$ are distributed according to Wigner semi-circle law,

$$\rho(J_\mu) = \frac{1}{2\pi} \sqrt{4 - J_\mu^2} \quad (4)$$

Denoting by ϕ_μ the spin coordinates in the basis that in which (J_{ij}) is diagonal, the Hamiltonian simplifies into

$$\beta\mathcal{H} = -\frac{\beta}{2N} \sum_\mu J_\mu \phi_\mu^2 + \frac{u}{N} \left(\sum_\mu \phi_\mu^2 \right)^2 \quad (5)$$

and the equation of motion now reads

$$\frac{\partial}{\partial t} \phi_\mu = \beta J_\mu \phi_\mu + 4u \phi_\mu \frac{1}{N} \sum_\nu \phi_\nu^2 + \eta_\mu(t) \quad (6)$$

where the η_μ 's are independent white Gaussian noises with variance 2.

B. Ferromagnetic model

It been remarked that the $p = 2$ spin glass resembles a ferromagnet 'in disguise' [24]. To illustrate this, we also consider a ferromagnetic model whose Hamiltonian \mathcal{H}_{FM} is given by

$$\beta\mathcal{H}_{\text{FM}} = -\beta \sum_{\langle ij \rangle} \sigma_i \sigma_j + \frac{u}{N} \sum_{i,j} \sigma_i^2 \sigma_j^2. \quad (7)$$

where the first sum runs over nearest neighbours on a d -dimensional (hyper)-cubic lattice, but the u -term retains interactions between all sites. (Thus, the model contains infinite-ranged couplings, as in the spherical ferromagnet.) The analogues of the co-ordinates ϕ_μ in this model are the Fourier transformed spin co-ordinates $\phi_{\mathbf{k}}$ where $\mathbf{k} = (k_1, \dots, k_d)$ is the wave vector. The eigenvalues of the matrix coupling the spins are $E_{\mathbf{k}} = \sum_{r=1}^d \cos k_r$. The resulting equation of motion is then

$$\frac{\partial}{\partial t} \phi_{\mathbf{k}} = \beta E_{\mathbf{k}} \phi_{\mathbf{k}} + 4u \phi_{\mathbf{k}} \frac{1}{N} \sum_{\mathbf{k}} |\phi_{\mathbf{k}}|^2 + \eta_{\mathbf{k}}(t) \quad (8)$$

where the $\eta_{\mathbf{k}}$ are independent Gaussian noises as before.

In $d = 3$ the distribution of the eigenvalues $E_{\mathbf{k}}$ is $\rho(E_{\mathbf{k}}) \approx (2\pi^2)^{-1} \sqrt{d - E_{\mathbf{k}}}$ when $|\mathbf{k}|$ is small. Similarly, in the spin glass of (1), the density of eigenvalues scales as $\rho(J_\mu) \approx \pi^{-1} \sqrt{(2 - J_\mu)}$ for J_μ close to 2. We will find that the phase transitions in the models depend on the scaling of the eigenvalue density near these points, and hence that phase transitions in the $d = 3$ ferromagnet and the $p = 2$ spin glass are related to each other, and have the same scaling exponents.

C. Symmetry-breaking fields

Below its transition temperature, the ferromagnetic model spontaneously breaks the global symmetry $\sigma_i \rightarrow -\sigma_i$. To clarify the behaviour in the ordered phase, it is convenient to introduce a magnetic field: we take $\mathcal{H}_{\text{FM}} \rightarrow \mathcal{H}_{\text{FM}} - h \sum_i \sigma_i$ in (7). The equation of motion becomes

$$\frac{\partial}{\partial t} \phi_{\mathbf{k}} = \beta(E_{\mathbf{k}} \phi_{\mathbf{k}} + h \delta_{\mathbf{k},0} \sqrt{N}) + 4u \phi_{\mathbf{k}} \frac{1}{N} \sum_{\mathbf{k}} |\phi_{\mathbf{k}}|^2 + \eta_{\mathbf{k}}(t) \quad (9)$$

In the presence of this field, the magnetisation $\mathcal{M}(t) = N^{-1} \sum_i \sigma_i = N^{-1/2} \phi_{\mathbf{k}=0}$ acquires a finite expectation

value: in the ordered phase, the magnetisation remains finite even in the limit of small h , with a first-order phase transition at $h = 0$.

In the spin glass model, the low temperature phase breaks the same global symmetry, but the order parameter is not the magnetisation. Instead, the co-ordinate ϕ_μ corresponding to the largest eigenvalue of J_{ij} becomes macroscopically occupied. We assign the label $\mu = 0$ to this eigenvector. Then, by analogy with the ferromagnetic case, we can introduce an analogous ‘staggered field’ to the model of (1). The equation of motion becomes

$$\frac{\partial}{\partial t}\phi_\mu = \beta(J_\mu\phi_\mu + h_s\delta_{\mu,0}\sqrt{N}) + 4u\phi_\mu \frac{1}{N} \sum_\nu \phi_\nu^2 + \eta_\mu(t) \quad (10)$$

The analogue of the magnetisation $\mathcal{M}(t)$ is the staggered magnetisation $\mathcal{M}_s(t) = N^{-1/2}\phi_{\mu=0}$. In the low temperature phase of the $p = 2$ spin glass, the expectation of $\mathcal{M}_s(t)$ tends to a finite value as h_s tends to zero, with a first-order phase transition at $h_s = 0$.

D. Thermodynamic formalism

Ruelle’s thermodynamic formalism involves a statistical mechanical analysis of the trajectories that a system follows through configuration space. Let a *history* be a particular time-realization that the system has visited over a given time interval. Consider an ensemble of histories constructed by fixing their dynamical activity $K(t)$. Here, the dynamical activity is a history-dependent observable, extensive both in space and time, expressing the amount of activity within the history. In a typical inactive history, the spins remain frozen in a locally ordered state; in an active history, spins fluctuate randomly between up and down states. For both spin-glass and ferromagnetic models, a simple local observable consistent with this definition of activity is

$$K(t) = -\frac{1}{2} \sum_j \int_0^t dt \sigma_j^2(t) = -\frac{1}{2} \sum_\mu \int_0^t dt \phi_\mu^2(t) \quad (11)$$

Histories with K close to 0 are the most active ones and are typically associated with disordered states; histories with large negative K are inactive and are associated either with local or global ordering.

While an ensemble of trajectories with fixed K is natural from a physical point of view, our theoretical methods require a change of ensemble, to one in which the average activity is fixed. (To draw an analogy with equilibrium statistical mechanics, we are transforming from a microcanonical to a canonical ensemble.) To fix the average activity, we apply a field s that is conjugate to $K(t)$. While we are as yet unable to endow s with an experimentally-realizable physical meaning, ensembles of histories with finite s provide a valuable theoretical tool, which allow us to probe the histories that the system follows. The ensemble with $s = 0$ is simply the (unbiased)

ensemble of trajectories for the system: ensembles with $s > 0$ are less active than the unbiased ensemble while those with $s < 0$ are more active.

In the following, we will evaluate the partition function

$$Z(s, t) = \langle e^{-sK} \rangle_0 \quad (12)$$

which is simply the generating function for the activity. Here and throughout, we use $\langle \cdot \rangle_0$ to denote an average of the (unbiased) relaxational dynamics over all possible time realizations, which means an average over the noises η_i . We also consider averages of a generic observable A in the biased ensemble parameterised by s , which we write as $\langle A \rangle_s \equiv \lim_{t \rightarrow \infty} Z^{-1}(s, t) \langle A e^{-sK} \rangle_0$

We also define a dynamical free energy

$$\psi(s) = \lim_{t \rightarrow \infty} \frac{\ln Z(s, t)}{t}. \quad (13)$$

It follows that

$$\langle K \rangle_s = -Nt \frac{d\psi}{ds} \quad (14)$$

With these definitions, singularities in $\psi(s)$ are the dynamical phase transitions of the system. Discontinuities in the derivatives of $\psi(s)$ will correspond to phase transitions between active and inactive phases. By analogy with equilibrium statistical mechanics, transitions with a jump in $\langle K \rangle_s$ are termed ‘first-order’ or ‘discontinuous’; otherwise the transition is termed ‘continuous’. More specifically, if $\langle K \rangle_s$ is continuous and the second derivative is discontinuous then we refer to the transition as ‘second-order’.

E. Functional integral formulation

To evaluate dynamical observables such as $\langle K \rangle_s$, we use the Janssen-De Dominicis functional-integral formulation [23], as in earlier studies such as Ref. [16]. The relaxational dynamics for the spin $\phi_\mu(t)$ is given by (6). Using a functional integral representation the dynamical, s -dependent partition function introduced in (12) becomes

$$Z(s, t) = \int \mathcal{D}\phi \mathcal{D}\bar{\phi} \exp \left[- \int_0^t dt' L(t') \right] \quad (15)$$

where, omitting time-dependence for brevity,

$$L = \sum_\mu \bar{\phi}_\mu \left(\partial_{t'} \phi_\mu - \beta J_\mu \phi_\mu + \frac{4u}{N} \sum_\nu \phi_\nu^2 \phi_\mu \right) - \bar{\phi}_\mu^2 - \frac{s}{2} \phi_\mu^2. \quad (16)$$

(We consider the spin-glass model of (1) and we have set the staggered field $h_s = 0$; other cases will be discussed below.)

Due to the infinite-ranged interactions in the term proportional to u , this model may be reduced to a quadratic

form. Details are given in appendix A. The result is that the partition function becomes

$$Z(s, t) = \int \mathcal{D}\phi \mathcal{D}\bar{\phi} \exp \left[8u\bar{\chi}\chi Nt - \int_0^t dt' L_{\text{aux}}(t') \right] \quad (17)$$

with

$$L_{\text{aux}} = \sum_{\mu} \bar{\phi}_{\mu} (\partial_{t'} + 4u\chi - \beta J_{\mu}) \phi_{\mu} - \bar{\phi}_{\mu}^2 - \left(\frac{s}{2} - 4u\bar{\chi} \right) \phi_{\mu}^2 \quad (18)$$

where the parameters χ and $\bar{\chi}$ must be determined self-consistently, through

$$\chi = \int dJ_{\mu} \rho(J_{\mu}) \frac{1}{\sqrt{(4u\chi - \beta J_{\mu})^2 - 2(s - 8u\bar{\chi})}} \quad (19)$$

and

$$2\bar{\chi} + 1 = \int dJ_{\mu} \rho(J_{\mu}) \frac{4u\chi - \beta J_{\mu}}{\sqrt{(4u\chi - \beta J_{\mu})^2 - 2(s - 8u\bar{\chi})}} \quad (20)$$

In addition, it follows from the definition of χ that

$$\chi = -2\langle K \rangle_s \quad (21)$$

so that solving the self-consistency equations (19) and (20) leads directly to the activities of the relevant phases. Finally, we note that the derivative

$$\frac{d\chi}{ds} = \langle (K - \langle K \rangle_s)^2 \rangle_s \quad (22)$$

gives the fluctuations of the activity.

Physically, we have shown that the dynamical correlation functions of the original model (1) are the same as those of the auxiliary quadratic system (17). Noting that $\rho(J_{\mu})$ is finite only for $-2 < J_{\mu} < 2$, the integrals in (19) and (20) are well-defined as long as

$$(4u\chi - 2\beta)^2 - 2(s - 8u\bar{\chi}) > 0 \quad (23)$$

As long as this condition is fulfilled, then the system is in a paramagnetic disordered phase. On the other hand, if the denominator of (19) vanishes at $J_{\mu} = 2$ then the mode associated with this eigenvalue may become macroscopically populated.

F. Symmetry-breaking fields

As discussed in Sec. II C, it is also useful to consider the effects of symmetry-breaking fields h_s and h on these systems. Following the analysis of the previous section, the symmetry-breaking fields lead to linear terms in L_{aux} . In general, the fluctuating magnetisation $\mathcal{M}_s = N^{-1/2} \bar{\phi}_{\mu=0}$ and its response field $\bar{\mathcal{M}}_s = N^{-1/2} \bar{\phi}_{\mu=0}$ both have finite expectation values which we denote by m_s and \bar{m}_s

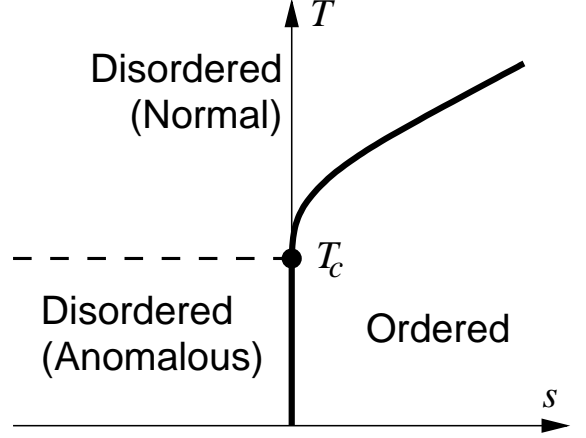


FIG. 1: ‘Phase diagram’ associated with the dynamic free energy $\psi(s)$ of the spin glass model. The critical point of the model is at $s = 0$ and $T = T_c$. The heavy solid line is a second order phase boundary between ordered and disordered phases. The dashed line is a crossover within the disordered phase. In the high temperature (normal) regime then the response to a staggered field h_s is positive; the low temperature (anomalous) regime is characterised by a negative response to this field.

respectively. Evaluating these expectation values in the auxiliary model, we arrive at

$$m_s = \beta h \frac{4u\chi - 2\beta}{(4u\chi - 2\beta)^2 - 2(s - 8u\bar{\chi})} \quad (24)$$

$$\bar{m}_s = \beta h \frac{s - 8u\bar{\chi}}{(4u\chi - 2\beta)^2 - 2(s - 8u\bar{\chi})}. \quad (25)$$

Self-consistency in the presence of the field leads to modified saddle point equations for χ and $\bar{\chi}$:

$$\chi = m_s^2 + \int \frac{dJ_{\mu} \rho(J_{\mu})}{\sqrt{(4u\chi - \beta J_{\mu})^2 - 2(s - 8u\bar{\chi})}} \quad (26)$$

$$2\bar{\chi} + 1 = 2m_s \bar{m}_s + \int \frac{dJ_{\mu} \rho(J_{\mu}) (4u\chi - \beta J_{\mu})}{\sqrt{(4u\chi - \beta J_{\mu})^2 - 2(s - 8u\bar{\chi})}}. \quad (27)$$

Finally we note that while we have considered the spin-glass model of (1) throughout Secs. II E and II F, the equations for the ferromagnetic model can be obtained by applying the simple replacement $(\mu, J_{\mu}, m_s, \bar{m}_s) \rightarrow (\mathbf{k}, E_{\mathbf{k}}, m, \bar{m})$ throughout these sections, where $\bar{m} = N^{-1/2} \bar{\phi}_{\mathbf{k}=0}$.

III. DESCRIPTION OF THE PHASE DIAGRAM

A. Overview

The dynamical phase diagram for the $p = 2$ spin glass of (1) is shown in Fig. 1, for $h_s = 0$. The phase diagram of the ferromagnetic model of (7) at $h = 0$ has the same

form. The axis $s = 0$ corresponds to the unbiased relaxational dynamics of (3). On this axis, the spin-glass system has a second-order phase transition at

$$T_c = \frac{1}{\sqrt{2u}}. \quad (28)$$

Below T_c , the mode with lowest eigenvalue is macroscopically populated, and the system is ordered: the (staggered) magnetisation remains finite as the (staggered) field is reduced to zero.

We will show that the effect of positive s is to promote ordering in the system, consistent with the expectation that ordered phases are less active than disordered ones. As s increased from zero, the second-order transition between active and inactive phases moves to a higher temperature: we have an increasing function $T_c(s)$, with $T_c(0) = T_c$ being the thermodynamic transition temperature at $s = 0$.

The effect of negative s is to reduce ordering in the system, thus increasing the activity: at temperatures above T_c , the dynamical free energy $\psi(s)$ has no singularities for $s \leq 0$ and K increases smoothly as s is decreased from zero. We also find that no ordered phases are possible for $s < 0$: the condition (23) is always satisfied when and m_s vanishes in the limit of small h_s . Thus, for $0 < T < T_c$, behaviour of the model as $s \rightarrow 0^+$ coincides with the ordered phase that is found at $s = 0$, but the behaviour is different for all $s < 0$. This signals the presence of a phase boundary at $s = 0$. The same effect is observed in the ferromagnetic model of (7).

We now show how this phase diagram is obtained from the solutions to the self-consistency equations (19) and (20). We calculate the saddle point average χ as a function of s and the other parameters of the model: this gives the activity of the phases of the model through (21). In addition, we also calculate the (s -dependent) staggered magnetisation m_s which gives additional insight into the phases of interest.

B. Unbiased dynamics ($s = 0$)

We begin with the unbiased ($s = 0$) behavior of the model, the derivation of which is identical to that of Kosterlitz *et al* [18] for the spherical version of this model. Equations (19) and (20) can be solved at $s = 0$ with the result that $\bar{\chi} = 0$, as required by causality, and that

$$\chi = \frac{1}{N} \sum_{\mu} \frac{1}{4u\chi - \beta J_{\mu}} \quad (29)$$

If $\chi > \frac{\beta}{2u}$ then we can approximate the sum over the eigenvalues J_{μ} by an integral over the distribution $\rho(J_{\mu})$, with the result

$$\chi = \frac{1}{\beta^2} \left(2u\chi - \sqrt{4u^2\chi^2 - \beta^2} \right) \quad (30)$$

the solution of which is given by

$$\chi = \frac{1}{\sqrt{4u - \beta^2}}, \quad \beta < \beta_c, \quad (31)$$

where $\beta_c = 1/T_c = \sqrt{2u}$ consistent with (28).

However, for $\beta > \beta_c$, the mode with $J_{\mu} = 2$ becomes macroscopically occupied, as described above. We therefore have

$$\chi = \frac{\beta}{2u}, \quad \beta > \beta_c. \quad (32)$$

While the integral in (19) is formally undefined, the ordered phase can be studied either by introducing a finite staggered field h_s as discussed in Sec. II F, or by solving (19) to $O(1/N)$. In either case, the staggered magnetisation m_s at zero field is

$$m_s = m_0 \equiv \sqrt{\frac{T_c^2 - T^2}{T}} \quad (33)$$

We also note a property of the ordered phase that is peculiar to exactly soluble soft spins models such as the spherical model [15]. The susceptibility associated with the magnetisation,

$$m^{(2)} = \langle (\mathcal{M}(t) - m_s)^2 \rangle_s \quad (34)$$

diverges as $h_s \rightarrow 0$ for the unbiased dynamics ($s = 0$) and all $T < T_c$. (This can be verified by evaluating $\langle \phi_0^2 \rangle$ in the auxiliary model.) This is in contrast to the usual situation in critical phenomena where $m^{(2)}$ is finite for zero field and $T < T_c$, diverging only at the critical point.

C. Ordered phase, $s > 0$

We now turn to the ordered phase for positive s . To simplify the analysis, we introduce reduced variables:

$$X(s) = 4uT\chi(s) \quad (35)$$

$$Y(s) = 2T^2[s - 8u\bar{\chi}(s)], \quad (36)$$

where we explicitly indicate the s -dependence of χ and $\bar{\chi}$. We see that $X(s) = \lambda^*$: physically, we identify the quantity $(-\lambda^*\phi_{\mu})$ in (A3) as the constraint force on mode μ that arises from the u -term in (1) and suppresses configurations with extreme values of ϕ_{μ} . We also identify $Y(s)$ as a renormalised field s for the auxiliary system. It is easily verified that while the dynamical free energy ψ depends on four parameters (s, β, u, h_s), the properties of the auxiliary model depends only on (Y, β, X, h_s) . Our strategy will be to determine properties of the auxiliary model in terms of X and Y and then to find the relations between (X, Y) and the bare parameters of the model.

In the presence of a staggered field h_s , we have from (26) that

$$m_s = h_s \frac{X - 2}{(X - 2)^2 - Y} \quad (37)$$

For $Y > 0$, spontaneous symmetry breaking occurs if the denominator vanishes as $h_s \rightarrow 0$, as

$$X = 2 + \sqrt{Y} + O(h_s). \quad (38)$$

Working at small h_s , we then take the zeroth order terms in (26), arriving at

$$\frac{2 + \sqrt{Y}}{4uT} = m_s^2 + T \int dJ \rho(J) \frac{1}{[2(2-J)\sqrt{Y} + (2-J)^2]^{1/2}} \quad (39)$$

This allows us to obtain $m_s^2 = m_0^2 + \frac{2\sqrt{2}T}{\pi} Y^{1/4} + O(Y^{1/2})$.

Finally, we must relate the renormalised field Y to the bare field s . Again working at zeroth order in h_s , (27) becomes:

$$\frac{2s - Y\beta^2}{8u} = \beta m_s^2 \sqrt{Y} - 1 + \int dJ \rho(J) \frac{2 - J + \sqrt{Y}}{[2(2-J)\sqrt{Y} + (2-J)^2]^{1/2}} \quad (40)$$

Taking s small and positive, the solution has small positive Y . More specifically, the first term on the right hand side of (40) dominates as $Y \rightarrow 0$, leading to $\sqrt{Y} = \frac{s}{2(\beta^2 - 2u)}$. [The same result can be obtained by working at $h_s = 0$ and considering carefully the limit of large- N . The analogue of (38) is $X = 2 + \sqrt{Y} + O(1/N)$ and we allow for a finite values of m_s and \bar{m}_s when solving (26) and (27). The remainder of the analysis follows.]

Taking everything together, in the limit $h_s \rightarrow 0^+$ and for $0 < s \ll (T - T_c)$, the leading behaviour is

$$\chi \approx \frac{\beta}{2u} + \frac{s\beta}{8u(\beta^2 - 2u)} \quad (41)$$

$$m_s^2 \approx m_0^2 + \frac{2}{\pi\beta} \sqrt{\frac{s}{\beta^2 - 2u}} \quad (42)$$

Physically, we can see that the $s = 0$ axis in the phase diagram of Fig. 1 is singular, but that both χ and $d\chi/ds$ are finite, so that fluctuations of the activity $K(t)$ remain finite as $h \rightarrow 0$. However, as for the case $s = 0$, the fluctuation $m^{(2)}$ diverges as $h \rightarrow 0$, for all cases where the spin-reversal symmetry is spontaneously broken.

D. High temperature regime

We now turn to temperatures above the critical temperature, $\beta < \beta_c$. We treat s perturbatively in (19) and (20), arriving at

$$\chi = \frac{1}{\sqrt{4u - \beta^2}} + s \frac{1}{8(2u - \beta^2)\sqrt{4u - \beta^2}} \quad (43)$$

noting also that

$$Y = 2s \frac{2u - \beta^2}{\beta^2(4u - \beta^2)}. \quad (44)$$

We also notice that these solutions satisfy $(X - 2)^2 - Y > 0$ at small s .

As the temperature is lowered towards T_c , we see that $d\chi/ds$ diverges. This again signals the second-order transition to the ordered phase. Indeed, it can be shown that this transition to the ordered phase moves to a higher temperature for $s > 0$. At the critical point, we have $(X - 2)^2 = Y$ and $m_s = \bar{m}_s = 0$. With these conditions, we can use (39) and (40) to derive the phase boundary for positive s . In the limit $\beta \rightarrow \beta_c^-$, the system is ordered for $s > s_c$, where

$$s_c(\beta) \simeq \frac{2\pi^2}{3\beta_c} (\beta_c - \beta)^3 \quad (45)$$

which holds to leading order in $\beta_c - \beta$. This function gives the phase boundary in Fig. 1, and its inverse gives the function $T_c(s)$ discussed above.

This completes our analysis of the phase diagram for $s \geq 0$. There is an ordered phase separated from a paramagnet by a second-order phase transition. Loosely, the effect of positive s is simply to stabilise the ordered phase, so that spontaneous symmetry breaking takes place at a higher temperature.

E. Anomalous paramagnetic regimes

We now take $s < 0$ but we remain in the low temperature regime with $\beta > \beta_c$. Working in terms of the reduced variables X, Y , we take $Y < 0$ so that we have

$$(X - 2)^2 - Y > 0, \quad (46)$$

and the integrand of (20) is finite for $-2 < J_\mu < 2$. To make progress with the integrals in (19,20): we define

$$I_1(X, Y) = \int dJ_\mu \rho(J_\mu) \frac{1}{\sqrt{(X - J_\mu)^2 - Y}}. \quad (47)$$

$$I_2(X, Y) = \int dJ_\mu \rho(J_\mu) \frac{(X - J_\mu)}{\sqrt{(X - J_\mu)^2 - Y}}. \quad (48)$$

We will consider the limit $Y \rightarrow 0^-$, in which the solution to (20) is $X \rightarrow 2^-$. The relevant limit is $0 < (-Y) \ll (2 - X)^2 \ll 1$. Writing $y' = -Y$ and $x' = 2 - X$, and after some manipulations presented in appendix B, we obtain:

$$I_1 = \pi^{-1} \sqrt{x'} \ln(4x'^2/y') + 1 + \frac{y'}{2x'^{3/2}} + O(x'^{1/2}) \quad (49)$$

$$I_2 = 1 - \frac{4(x')^{3/2}}{3\pi} + O(y'x'^{-1/2}) + O(x'^{5/2}) \quad (50)$$

The self-consistent equation (19) takes the form

$$\frac{\beta^2}{4u} (2 - x') = 1 + \frac{\sqrt{x'}}{\pi} \ln \frac{4x'^2}{y'} + o(1), \quad (51)$$

where we define $o(1)$ terms as quantities which vanish for $y \ll x'^2 \ll 1$. Recalling that $X = 2 - x' = 4uT\chi$, we have to leading order

$$\chi \approx \frac{\beta}{4u} \left(2 - \frac{\pi^2}{4u^2} \frac{(\beta^2 - 2u)^2}{\ln^2(-1/Y)} \right). \quad (52)$$

Then, substituting for x' in (50) and recalling (20), we have

$$\bar{\chi} \approx -\frac{\pi^2}{12u^3} \frac{(\beta^2 - 2u)^3}{\ln^3(-1/Y)}. \quad (53)$$

Noting that $y' = -2T^2(s - 8u\bar{\chi})$ we see that when $s \rightarrow 0$, $\bar{\chi} \gg y'$, so that $s \simeq 8u\bar{\chi} + o(1)$. This simplifies the expressions for χ and $\bar{\chi}$ which become:

$$\chi \approx \frac{\beta}{2u} \left[1 - \left(\frac{3\pi}{16u} \right)^{\frac{2}{3}} (-s)^{\frac{2}{3}} \right] \quad (54)$$

$$\bar{\chi} \approx \frac{s}{8u} \quad (55)$$

which hold at leading order in $s < 0$ and for $\beta > \beta_c$.

We refer to the phase with $s < 0$ and $T < T_c$ as an anomalous disordered phase. To understand this terminology, it is useful to consider the linear response to the field h_s , which is given by (24). Since we have $0 \ll -Y \ll (2 - X)^2$ with $X > 2$, this reduces to

$$m_s = \frac{-h_s}{2 - X} \quad (56)$$

We can see that the response to the staggered field is a staggered magnetisation in the opposite direction (a diamagnetic response). In addition, it follows from (54) that $dm_s/dh_s \sim -|s|^{-2/3}$ for $s \rightarrow 0^-$. That is, the diamagnetic response diverges. Clearly such a response would be impossible in the unbiased ($s = 0$) ensemble due to thermodynamic convexity arguments, but when considering ensembles with finite s then such arguments do not apply.

Finally, we consider the nature of the phase transition between ordered and anomalous disordered phases. Comparing (41) and (54), we note that χ is continuous at $s = 0$, and hence that the activity $\langle K \rangle_s$ is continuous also. Thus, we identify a continuous phase transition at $s = 0$, consistent with Fig. 1. Often, at continuous phase transitions, one may identify a path between the phases along which the free energy is analytic and which remains always near the critical point. (For example, in a ferromagnet one can move between ordered and disordered phases by applying a small field h , decreasing the temperature and then removing the field.) However, in the transition considered here, the (staggered) magnetisation m_s is zero for $s < 0$ but has a finite limit as $s \rightarrow 0^+$. This seems to preclude such a route around the critical point. Further, evaluating $(d\chi/ds)$ indicates that the fluctuations of the activity diverge as $s \rightarrow 0^-$ but remain finite as $s \rightarrow 0$. This also indicates the absence of a path between the phases that is continuous near the transition.

We turn to this issue in the next section, where we also discuss the possibility of diverging length scales near this transition.

F. Effect of the staggered field h_s on disordered phases

To understand the behaviour near this phase transition in more detail, we introduce a finite staggered field $h_s > 0$ and note that the crossover between normal ($m_s > 0$) and anomalous ($m_s < 0$) behaviour takes place at $\chi = \beta/2u$. If we insist that χ take this value, the self-consistency equation (26) becomes

$$\int dJ_\mu \rho(J_\mu) \frac{1}{\sqrt{(2 - J)^2 - Y}} = (\beta/\beta_c)^2 \quad (57)$$

For $\beta < \beta_c$ (high temperatures), this equation has a unique solution for $Y < 0$, which signals a crossover from normal to anomalous behaviour, at a value of Y that is independent of the field h_s . On the other hand, in the low temperature regime $\beta > \beta_c$, (57) has no solutions.

One may verify that for large positive s , the solution of (26) has $X \rightarrow 0$, while for small positive s we have from (41) that $X > 2$. Since (57) establishes that, for low temperatures, there are no values of Y for which $X = 2$, it follows that the s -dependent value of X has a jump from a value greater than 2 to a value smaller than 2. This is a discontinuous phase transition from normal to anomalous states. (The field h_s is finite, so the concept of a spontaneously ordered state is not useful. However, the sign of the staggered magnetisation is positive in the normal state and negative in the anomalous one.) These arguments lead us to propose the qualitative phase diagram shown in Fig. 2. The presence of first-order transitions at finite h_s explains the unusual features of the order-disorder transition at $s = h_s = 0$: there are indeed no continuous paths between the ordered and disordered states due to the first order transition at finite h_s .

The nature of the scaling behaviour near T_c in this model is clearly complicated, depending qualitatively on the order in which s , h_s and $T - T_c$ are taken to zero, and also on the signs of s and $T - T_c$. A detailed investigation of these finite- h_s transitions is beyond the scope of this paper. However, we can conclude that the order-disorder transition at $h_s = s = 0$ is second-order in that $\chi(s)$ is continuous, but that the spontaneous staggered magnetisation m_s goes discontinuously to zero at this transition. We again emphasise that all of this phenomenology is also present in the ferromagnetic model of (7), at least for $d = 3$. We expect the qualitative features to also be present in higher dimensions.

In the ferromagnetic model, we can also consider the correlation lengths of the various phases. These appear through the \mathbf{k} -dependence of the fluctuations:

$$S(\mathbf{k}, s) \equiv \langle |\phi_{\mathbf{k}}|^2 \rangle_s = \frac{T}{\sqrt{(X - E_{\mathbf{k}})^2 - Y}} \quad (58)$$

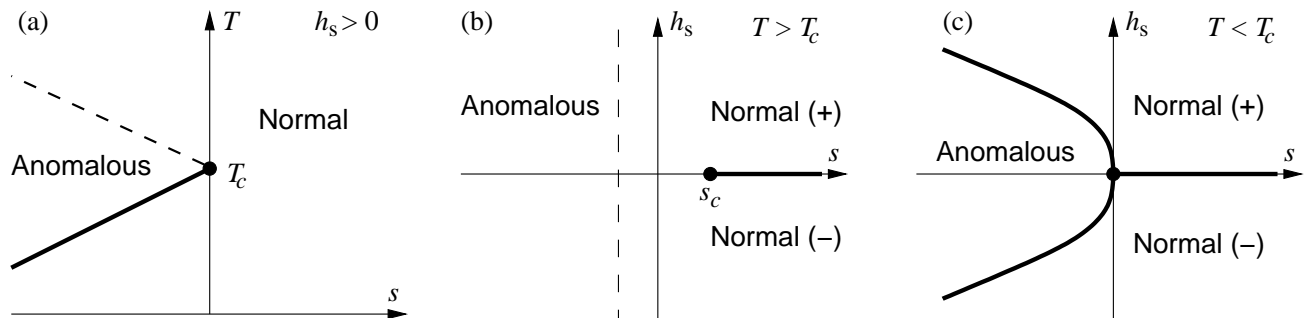


FIG. 2: (a) Proposed phase diagram for $h_s > 0$. The solid line is a first-order phase transition at which the staggered magnetisation and the activity X are discontinuous. It ends at a critical point at $T = T_c$ and $s = 0$, but we note that h_s is finite at this critical point. The dashed line is a crossover at which the linear response to a staggered field h_s vanishes. The dashed line is independent of h_s while the solid line approaches the $s = 0$ axis as $h_s \rightarrow 0$. (b) Behaviour as a function of the field h_s in the high temperature regime. For negative s , there is a crossover from normal to anomalous response: at the crossover $X = 2$ and Y satisfies (57). For positive s , there is a critical point at s_c , with spontaneous symmetry breaking for $s > s_c$. Close to T_c , the critical value of s_c is given by (45). (c) Behaviour as a function of h_s in the low temperature regime. The solid line for $s < 0$ is a first-order phase transition between states with positive and negative response to the staggered field, while the line for $s > 0$ is the usual first-order transition between spontaneously-ordered states.

Recall that $E_{\mathbf{k}} \leq d$ with equality if $\mathbf{k} = 0$.

Two cases are of interest. Firstly, if the denominator vanishes at $\mathbf{k} = 0$ as in the ordered states, the fluctuations of the spontaneous magnetisation diverge, as described above. Secondly, if $X < d$ as in the anomalous phase then $S(\mathbf{k})$ has a peak at a finite wave-vector \mathbf{k}^* for which $E_{\mathbf{k}^*} = X$. We interpret $1/|\mathbf{k}^*|$ as a characteristic length scale for structures within this phase. It is interesting to note that this length scale diverges as $s \rightarrow 0^-$ in the anomalous phase, and that this is accompanied by a divergence in the fluctuations of the spontaneous magnetisation [it may be easily verified that $S(\mathbf{0}, s \rightarrow 0^-)$ is divergent since $X \rightarrow d^-$ and $Y \rightarrow 0^-$ in this limit, by analogy with the $p = 2$ spin glass].

IV. INTERPRETATION

We have considered in some detail the large deviations of the dynamical activity in two soft-spin models. We end with a comparison with previous studies and with some comments on the relation between the large deviations that we studied and the phase behaviour of the models.

Based on the close relationship between the ferromagnetic and spin glass models, the form of the phase diagram in Fig. 1 is perhaps not too surprising: a similar result was found in Ref. [11] for the infinite-ranged (mean-field) Ising model. The equilibrium critical point leads to a dynamical phase transition at $s = 0$ below the critical temperature. However, instead of being first order as in the fully-connected model, the phase transition we have found is second order. Unlike the fully-connected models, the ferromagnetic model of (7) has several diverging length scales, although the presence of a diverging length scale throughout the ordered phase may be a peculiarity of our particular model. In any case, the diverging length

scale as $s \rightarrow 0^-$ within the anomalous phase seems to be a new feature that merits further investigation.

In particular, the existence of the anomalous phase seems to be linked to the existence of aging/coarsening solutions to the relaxational dynamics of these models. These solutions are characterised by $m_s = 0$ as in the anomalous phase and exhibit a length scale that grows with the time that has elapsed since a quench from above T_c . It can be readily shown that if multiple solutions to the equations of motion exist with different activity, then the field s acts to select the solutions with the larger ($s > 0$) or smaller ($s < 0$) activity, leading to a transition at $s = 0$. However, while the aging dynamics of the $p = 2$ spin-glass of (1) can be solved [25] by a similar method to that of Cugliandolo and Dean [20], we have not yet established any clear connection between these dynamics and the anomalous disordered phases discussed here. This too remains an area for future study.

We also compare the results shown here with those obtained for kinetically constrained models [12]. In both cases, active and inactive phases coexist at the $s = 0$ axis. However, there are two important differences. Firstly, in the kinetically constrained models considered in [12], the transition is first-order, signalling the coexistence of active and inactive solutions to the equations of motion. These have been interpreted as “ergodic fluid” and “non-ergodic glass” states [7, 8, 12, 13]. On the other hand, the continuous transition in the soft spin models is second order: the anomalous phase is characterised by a diverging correlation length that we have tentatively attributed to the growing length scale associated with the aging behaviour of the system. Taking the large-time limit of the aging solution, the activity of the system approaches that of the ordered state: the active (aging) and inactive (ordered) phase are not separated by a gap in the activity, unlike the kinetically constrained models.

Secondly, we emphasise that in the kinetically con-

strained models, the $s = 0$ axis of the phase diagram belongs to the active phase. Introducing any $s > 0$ leads immediately to an inactive phase that is qualitatively different from the unbiased state at $s = 0$. On the other hand, in the models considered here, the $s = 0$ axis belongs to the inactive (ordered phase): it is the introduction of any $s < 0$ that leads to an active phase that differs from the unbiased steady state.

Finally we note that contrary to its $p \geq 3$ counterparts, the thermodynamic properties of the $p = 2$ spin glass have only a single transition temperature and do not display any kind of replica symmetry breaking. Here, we have analysed this problem by diagonalising the quadratic dynamical action: a method that applies only for $p = 2$. However, the same results can be verified using the replica trick and integrating out the disorder. The application of such methods to models with $p \geq 3$ would provide further insight into the behaviour of large deviations of the activity in ‘glassy’ models.

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APPENDIX A: SADDLE-POINT INTEGRATION OF THE DYNAMICAL ACTION

Here, we show how the functional integral (15) can be cast in the form (17). We define

$$\mathcal{X}(t) = \frac{1}{N} \sum_{\mu} \phi_{\mu}^2(t), \quad (\text{A1})$$

which is proportional to the growth rate of the activity K defined in (11), and the related quantity:

$$\bar{\mathcal{X}}(t) = \frac{1}{N} \sum_{\mu} \bar{\phi}_{\mu}(t) \phi_{\mu}(t). \quad (\text{A2})$$

Both \mathcal{X} and $\bar{\mathcal{X}}$ are self-averaging quantities in the thermodynamic limit of large N . It is therefore convenient to constrain these quantities with Lagrange multipliers and then to integrate over these constrained quantities by a saddle-point method. Writing the (time-dependent) Lagrange multipliers as $\lambda, \bar{\lambda}$, Eq. (15) becomes:

$$Z(s, t) = \int \mathcal{D}\mathcal{X} \mathcal{D}\bar{\mathcal{X}} \frac{N \mathcal{D}\bar{\lambda}}{2\pi i} \frac{N \mathcal{D}\lambda}{2\pi i} \mathcal{D}\phi \mathcal{D}\bar{\phi} \left[e^{-N S_0(t) - S_1(t)} \right] \quad (\text{A3})$$

with

$$S_0(t) = \int_0^t dt' [\bar{\lambda}(t') \mathcal{X}(t') + \lambda(t') \bar{\mathcal{X}}(t') + 4u \mathcal{X}(t') \bar{\mathcal{X}}(t')] \quad (\text{A4})$$

and

$$S_1(t) = \int_0^t dt' \sum_{\mu} \left\{ \bar{\phi}_{\mu} \left[\frac{\partial}{\partial t'} + \lambda(t') - \beta J_{\mu} \right] \phi_{\mu} - \left[\frac{s}{2} + \bar{\lambda}(t') \right] \phi_{\mu}^2 - \bar{\phi}_{\mu}^2 \right\} \quad (\text{A5})$$

where we again omit the dependence of the fields ϕ and $\bar{\phi}$ on the time t' , for brevity.

In the $N \rightarrow \infty$ limit, the integrals over \mathcal{X} , $\bar{\mathcal{X}}$, λ and $\bar{\lambda}$ can be carried out through a saddle point approximation. We replace $\mathcal{X}(t)$, $\bar{\mathcal{X}}(t)$, $\lambda(t)$ and $\bar{\lambda}(t)$ by their saddle-point values χ , $\bar{\chi}$, λ^* and $\bar{\lambda}^*$. In particular, differentiating the action ($N S_0 + S_1$) with respect to \mathcal{X} and $\bar{\mathcal{X}}$, we arrive at

$$\bar{\lambda}^* = -4u \bar{\chi} \quad (\text{A6})$$

$$\lambda^* = -4u \chi. \quad (\text{A7})$$

Thus, performing the saddle-point integrals in (A3) leads to (17) in the main text. Similarly, differentiating with respect to λ and $\bar{\lambda}$ leads to the self-consistency equations (19) and (20).

APPENDIX B: COMPUTATION OF χ IN THE LOW-TEMPERATURE DISORDERED PHASE

Here we discuss the solutions of the self-consistency equations (19) and (20) for $s < 0$ and $T < T_c$. Using the notation of Sec. III E, we can write the integrals of Eqs. (47) and (48) as

$$I_1 = \int_{-4+x'}^{x'} \frac{dz}{2\pi} \frac{\sqrt{4(x'-z) - (x'-z)^2}}{\sqrt{z^2 + y'}} \quad (\text{B1})$$

$$I_2 = \int_{-4+x'}^{x'} \frac{dz}{2\pi} \frac{-z \sqrt{4(x'-z) - (x'-z)^2}}{\sqrt{z^2 + y'}} \quad (\text{B2})$$

Since we are at $\beta > \beta_c$ and $s < 0$, we have $x', y' > 0$. The small s limit becomes the limit $y' \rightarrow 0$ but if we take the limit for $y' \rightarrow 0$ keeping $x' > 0$ we have $I_1(x', y' \rightarrow 0) \rightarrow \infty$, and the self-consistency condition cannot be satisfied. We therefore take both x' and y' to zero together: we assume that $y' \ll x'^2$ which can be verified *a posteriori* through the solution to (51). The result is $x' \sim [\ln(1/y')]^{-2}$, consistent with our assumptions.

We start by splitting the integral in (B1) into three

parts:

$$\begin{aligned}
I_1 = & \int_{-x'}^{x'} \frac{dz}{2\pi} \frac{\sqrt{x'(4-x')}}{\sqrt{y'+z^2}} \\
& + \int_{-x'}^{x'} \frac{dz}{2\pi} \frac{\sqrt{4(x'-z)-(x'-z)^2} - \sqrt{x'(4-x')}}{\sqrt{z^2+y'}} \\
& + \int_{x'-4}^{-x'} \frac{dz}{2\pi} \frac{\sqrt{4(x'-z)-(x'-z)^2}}{\sqrt{z^2+y'}}. \quad (B3)
\end{aligned}$$

In the limit of $y' \ll x'^2$, the first integral has a divergent contribution $(\sqrt{x'}/\pi) \ln(4x'^2/y')$. In the second and third parts we can take the limit $y' \rightarrow 0$ directly in the integrand. If we then take the limit of small x' then we find that the second integral vanishes as $O(\sqrt{x'})$ while the third approaches unity. Thus we arrive at (49).

We now evaluate the $(y'/x'^2) \rightarrow 0$ limit of the expression (B2). We use a similar method, splitting the integral into two terms:

$$\begin{aligned}
I_2 = 1 + & \int_{-x'}^{x'} \frac{dz}{2\pi} \sqrt{4(x'-z)-(x'-z)^2} \left(\frac{-z}{\sqrt{z^2+y'}} - 1 \right) \\
& + \int_{x'-4}^{-x'} \frac{dz}{2\pi} \sqrt{4(x'-z)-(x'-z)^2} \left(\frac{-z}{\sqrt{z^2+y'}} - 1 \right). \quad (B4)
\end{aligned}$$

In the first integral we introduce $w = z/x'$ and $\sigma = y'/x'^2$, thus arriving at

$$(x')^{3/2} \int_{-1}^1 \frac{dw}{2\pi} \left(\frac{-w}{\sigma + w^2} - 1 \right) \sqrt{4(1-w) - x'(1-w)^2}. \quad (B5)$$

The leading behaviour of this quantity can be evaluated by setting directly $\sigma = x' = 0$ into the integral, so that this contribution to I_2 is $-4(x')^{3/2}/(3\pi)[1 + o(1)]$.

For the second integral in Eq. (B4), we have $z^2 \geq x'^2$ so we expand the integrand in powers of $\sigma = y'/z^2$. The leading term vanishes and the second term is $O(y'/\sqrt{x'})$. Writing $(y'/\sqrt{x}) = (x')^{3/2}(y'/x'^2)$, this term is smaller first term in (B4) which is $O((x')^{3/2})$. Thus we arrive at

$$I_2 \approx 1 - \frac{4(x')^{3/2}}{3\pi}. \quad (B6)$$

as given in Equ. (50) of the main text.

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